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STRUCTURE FILE UPDATES: 10 DEC 2009 HIGHEST RN 1196958-61-8
DICTIONARY FILE UPDATES: 10 DEC 2009 HIGHEST RN 1196958-61-8

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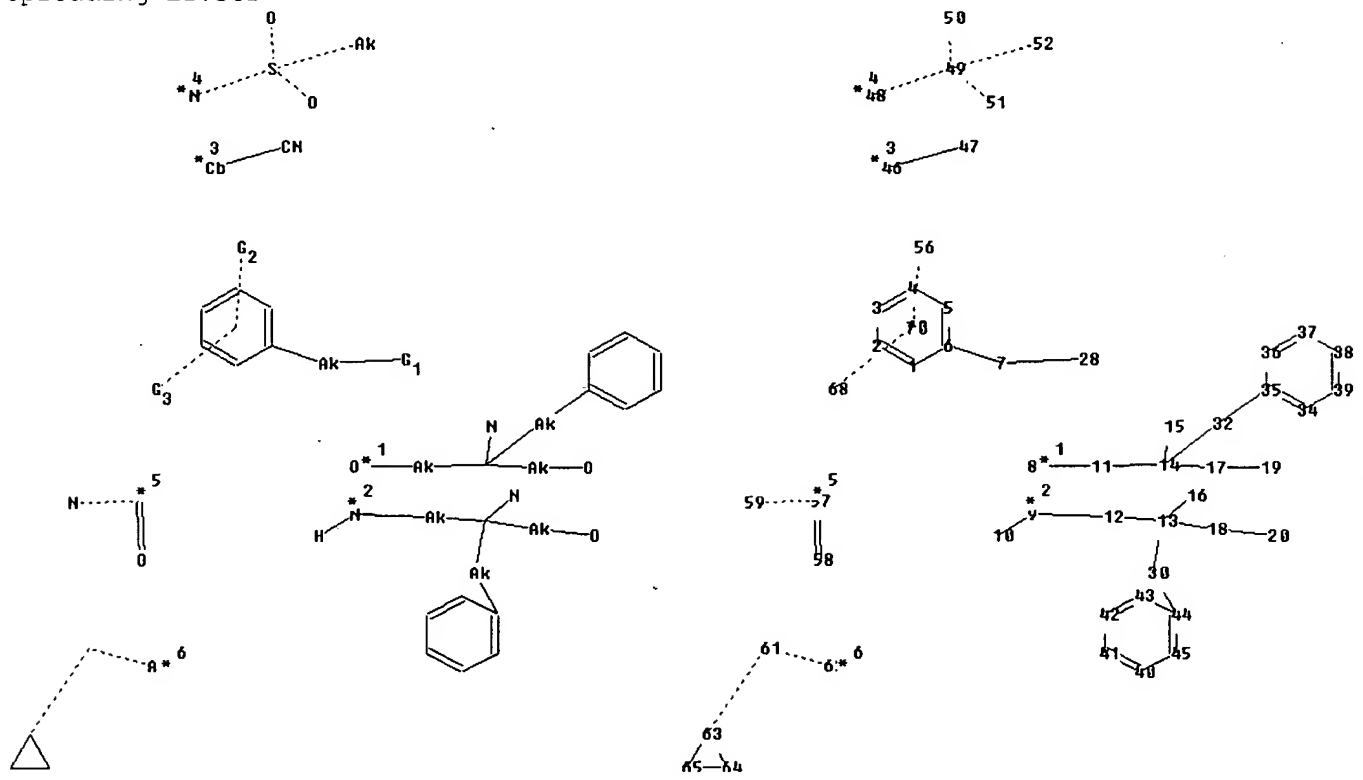
TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html
Uploading L1.str



chain nodes :
7 8 9 10 11 12 13 14 15 16 17 18 19 20 28 30 32 46 47 48 49 50 51 52 56 57 58 61 62 68
ring nodes :
1 2 3 4 5 6 34 35 36 37 38 39 40 41 42 43 44 45 63 64 65
ring/chain nodes :
59
chain bonds :
6-7 7-28 8-11 9-10 9-12 11-14 12-13 13-16 13-18 13-30 14-15 14-17 14-32 17-19 18-20 30-44 32-35 46-47 48-49 49-50 49-51 49-52 57-58 57-59 61-62 61-63
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 34-35 34-39 35-36 36-37 37-38 38-39 40-41 40-45

```
41-42  42-43  43-44  44-45  63-64  63-65  64-65
exact/norm bonds :
6-7  7-28  8-11  9-12  11-14  12-13  13-16  13-18  13-30  14-15  14-17  14-32  30-
44
32-35  48-49  49-50  49-51  49-52  57-58  57-59  61-62  61-63  63-64  63-65  64-65
exact bonds :
9-10  17-19  18-20  46-47
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  34-35  34-39  35-36  36-37  37-38  38-39  40-41  40-
45
41-42  42-43  43-44  44-45


G1:[*1],[*2]

G2:[*3],[*4]

G3:[*5],[*6]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS
19:CLASS  20:CLASS
28:CLASS  30:CLASS  32:CLASS  34:Atom  35:Atom  36:Atom  37:Atom  38:Atom  39:Atom
40:Atom  41:Atom
42:Atom  43:Atom  44:Atom  45:Atom  46:Atom  47:CLASS  48:CLASS  49:CLASS  50:CLASS
51:CLASS
52:CLASS  56:CLASS  57:CLASS  58:CLASS  59:CLASS  61:CLASS  62:CLASS  63:Atom
64:Atom  65:Atom
68:CLASS  69:CLASS  70:CLASS
Generic attributes :
7:
Saturation              : Saturated
11:
Saturation              : Saturated
12:
Saturation              : Saturated
17:
Saturation              : Saturated
18:
Saturation              : Saturated
30:
Saturation              : Saturated
32:
Saturation              : Saturated

Element Count :
Node 7: Limited
    C,C1-2

Node 11: Limited
    C,C1-2

Node 12: Limited
    C,C1-2

Node 17: Limited
    C,C1-2

Node 18: Limited
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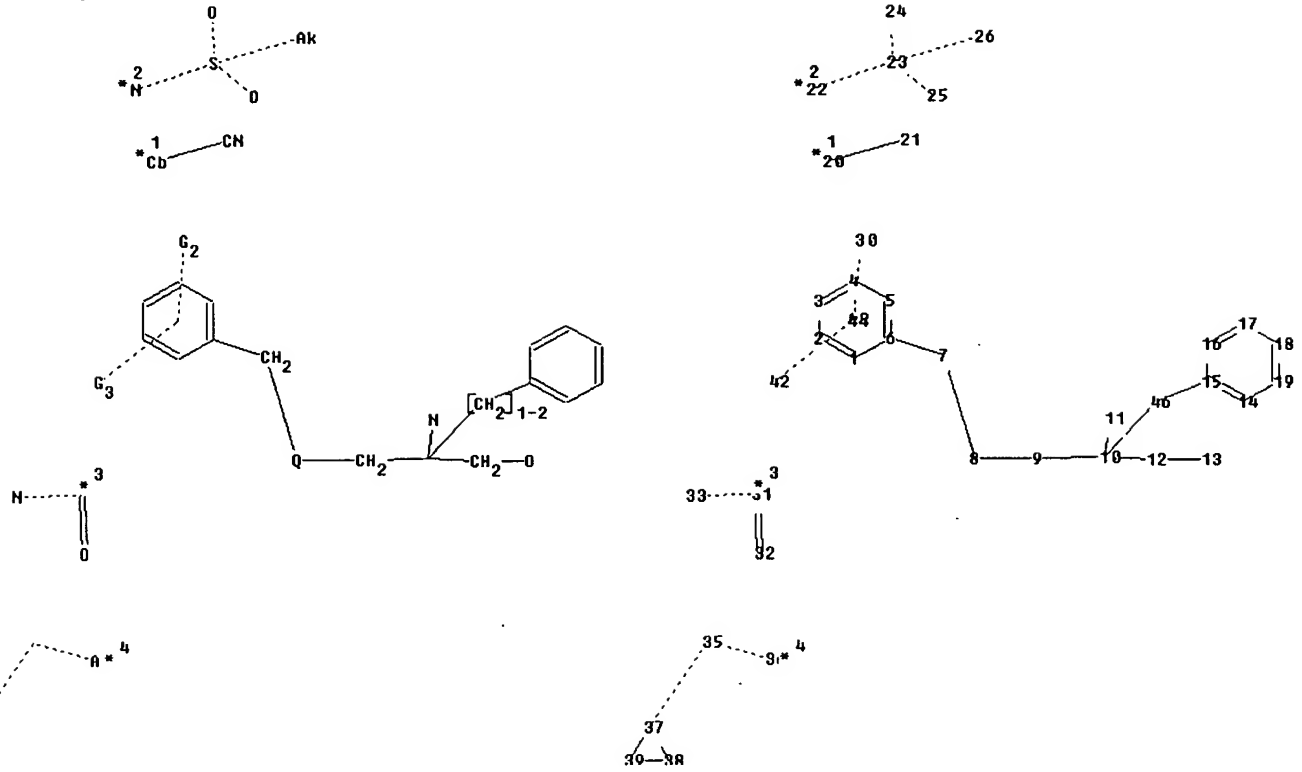
C,C1-2

Node 30: Limited
C,C1-3

Node 32: Limited
C,C1-3

Uploading L14.str



chain nodes :
7 8 9 10 11 12 13 20 21 22 23 24 25 26 30 31 32 35 36 42 46

ring nodes :
1 2 3 4 5 6 14 15 16 17 18 19 37 38 39
ring/chain nodes :
33
chain bonds :
6-7 7-8 8-9 9-10 10-11 10-12 10-46 12-13 15-46 20-21 22-23 23-24 23-25
23-26 31-32 31-33 35-36 35-37
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19 37-38 37-
39
38-39
exact/norm bonds :
7-8 8-9 10-11 22-23 23-24 23-25 23-26 31-32 31-33 35-36 35-37 37-38 37-
39
38-39
exact bonds :
6-7 9-10 10-12 10-46 12-13 15-46 20-21

normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19

G2:[*1],[*2]

G3:[*3],[*4]

Connectivity :
8:2 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:CLASS
22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 30:CLASS 31:CLASS 32:Atom
33:Atom 35:CLASS 36:CLASS
37:Atom 38:Atom 39:Atom 42:CLASS 43:CLASS 44:CLASS 46:CLASS

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FILE COVERS 1907 - 11 Dec 2009 VOL 151 ISS 25
FILE LAST UPDATED: 10 Dec 2009 (20091210/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

ZCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2009.

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This file contains CAS Registry Numbers for easy and accurate
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'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L6
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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L3              SCR 1071
L5           38 SEA FILE=REGISTRY SSS FUL L1 AND L3
L6            4 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L5


=> file beilstein
FILE 'BEILSTEIN' ENTERED AT 13:25:02 ON 11 DEC 2009
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FILE LAST UPDATED ON April 24, 2009

FILE COVERS 1779 TO 2008.
*** FILE CONTAINS 10,593,281  SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

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=> d stat que L8
L1              STR

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Structure attributes must be viewed using STN Express query preparation.
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L8            3 SEA FILE=BEILSTEIN SSS FUL L1 AND L3

100.0% PROCESSED    4773 ITERATIONS                          3 ANSWERS
SEARCH TIME: 00.00.08


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FILE 'WPIX' ENTERED AT 13:25:10 ON 11 DEC 2009
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FILE LAST UPDATED:          4 DEC 2009   <20091204/UP>
MOST RECENT UPDATE:           200978      <200978/DW>
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>>> IPC, ECLA, US National Classifications and Japanese F-Terms
    and FI-Terms have been updated with reclassifications to
    end of September 2009.
    No update date (UP) has been created for the reclassified
    documents, but they can be identified by
    specific update codes (see HELP CLA for details) <<<

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http://www.stn-international.com/DWPIAnaVist2_0608.html

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

>>> Japanese FI-TERM thesaurus in field /FCL added --> see NEWS <<<
'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> d stat que L11
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
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L10          27 SEA FILE=WPIX SSS FUL L1 AND L3
L11           2 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L10/DCR


=> file marpat
FILE 'MARPAT' ENTERED AT 13:25:20 ON 11 DEC 2009
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FILE CONTENT: 1961-PRESENT VOL 151 ISS 23 (20091204/ED)

MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US  20090275099 05 NOV 2009
DE 102008019858 22 OCT 2009
EP      2110127 21 OCT 2009
JP   2009260249 05 NOV 2009
WO   2009135699 12 NOV 2009
GB      2459133 14 OCT 2009
FR      2930141 23 OCT 2009
RU      2370496 20 OCT 2009
CA      2653107 08 AUG 2009

The new MARPAT User Guide is now available at:
 http://www.cas.org/support/stngen/stndoc/marpat.html.
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=> d stat que L16
L14             STR

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Structure attributes must be viewed using STN Express query preparation.
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100.0% PROCESSED  132230 ITERATIONS                              1 ANSWERS
SEARCH TIME: 00.00.40


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DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.
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PROCESSING COMPLETED FOR L6
PROCESSING COMPLETED FOR L8
PROCESSING COMPLETED FOR L11
PROCESSING COMPLETED FOR L16
L17           7 DUP REM L6 L8 L11 L16 (3 DUPLICATES REMOVED)
                ANSWERS '1-4' FROM FILE ZCAPLUS
                ANSWERS '5-7' FROM FILE BEILSTEIN

=> d ibib abs hitstr L17 1-4; d ide allref L17 5-7

L17  ANSWER 1 OF 7  ZCAPLUS  COPYRIGHT 2009 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2005:324002  ZCAPLUS  Full-text
DOCUMENT NUMBER:          142:373552
TITLE:                    Benzyl ethers and benzylamines as beta-secretase
                          inhibitors, their preparation and use for the
                          treatment of Alzheimer's disease
INVENTOR(S):              Nantermet, Philippe G.; Rajapakse, Hemaka Anthony;
                          Selnick, Harold G.
PATENT ASSIGNEE(S):       Merck & Co., Inc., USA
SOURCE:                   PCT Int. Appl., 47 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.        DATE
     ---------------      ----   --------    --------------------   --------
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| | | | | | |
|---|---|---|---|---|---|
| WO 2005032471 | A2 | 20050414 | WO 2004-US32009 | | 20040929 |
| WO 2005032471 | A3 | 20050707 | | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

| | | | | | |
|---|---|---|---|---|---|
| AU 2004277981 | A1 | 20050414 | AU 2004-277981 | | 20040929 |
| AU 2004277981 | B2 | 20091001 | | | |
| CA 2540452 | A1 | 20050414 | CA 2004-2540452 | | 20040929 |
| EP 1673078 | A2 | 20060628 | EP 2004-789263 | | 20040929 |
| EP 1673078 | B1 | 20080528 | | | |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

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|---|---|---|---|---|---|
| CN 1859904 | A | 20061108 | CN 2004-80028599 | | 20040929 |
| JP 2007507515 | T | 20070329 | JP 2006-534062 | | 20040929 |
| AT 396973 | T | 20080615 | AT 2004-789263 | | 20040929 |
| IN 2006DN01546 | A | 20070810 | IN 2006-DN1546 | | 20060322 |
| US 20060293380 | A1 | 20061228 | US 2006-573232 | | 20060323 |
| PRIORITY APPLN. INFO.: | | | US 2003-508369P | P | 20031003 |
| | | | WO 2004-US32009 | W | 20040929 |

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 142:373552
GI


* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

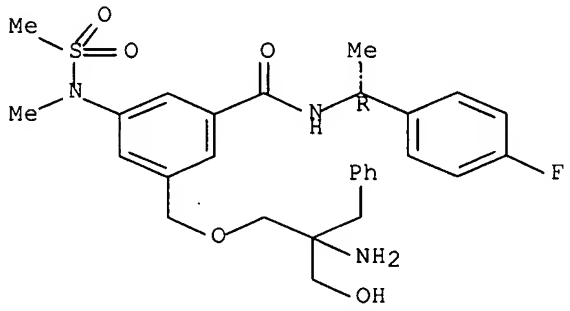

AB The invention relates to a group of benzyl ethers and benzylamines I which are inhibitors of the beta-secretase enzyme. In compds. I, X is O or NH; Y is CH or N; R1 is selected from aryl, arylmethyl, heterocyclyl, and heterocyclylmethyl, wherein the ring is unsubstituted or substituted with one or more substituents selected from halo, OH, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, cyano, and C1-6 alkoxy; R2 is selected from alkyl(alkylsulfonyl)amino, (alkylsulfonyl)amino, o-cyanophenyl, and, gem-cyanocycloalkyl; R3 is selected from (un)substituted (arylalkyl)aminocarbonyl, aminocarbonyl, alkylaminocarbonyl, cyclopropylethenyl, cyclopropylmethyloxy, and cyclopropylmethylamino; and includes all pharmaceutically acceptable salts. The invention also relates to the preparation of I, pharmaceutical compns. comprising these compds. and a pharmaceutically acceptable carrier, and the use of these compds. and compns. in the treatment of diseases in which the beta-secretase enzyme is involved, such as Alzheimer's disease. N-Methylsulfonylation of di-Me 5-aminoisophthalate, followed by N-methylation, gave II, which was partially hydrolyzed and coupled with a chiral amine to give III. Hydrolysis of III followed by borane reduction, bromination, and substitution with 2-amino-2-benzylpropane-1,3-diol, prepared by reduction of racemic α-benzylserine, resulted in the formation of IV. The compds. of the invention inhibit the beta-secretase enzyme, generally with IC50 values from about 1 nM to 100 μM.


IT **849622-98-6P**, 3-[(2-Amino-2-benzyl-3-hydroxypropoxy)methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]benzamide
**849623-02-5P**, 3-[[(2-Amino-2-benzyl-3-hydroxypropyl)amino]methyl]-

N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]benzamide trifluoroacetate 849623-03-6P, 3'-[(2-Amino-2-benzyl-3-hydroxypropoxy)methyl]-5'-[[2-(2-furyl)pyrrolidin-1-yl]carbonyl]-1,1'-biphenyl-2-carbonitrile 849623-05-8P **849623-06-9P 849623-07-0P 849623-08-1P 849623-09-2P 849623-10-5P 849623-11-6P 849623-12-7P 849623-13-8P 849623-14-9P 849623-15-0P 849623-16-1P 849623-18-3P 849623-19-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzyl ethers and benzylamines as beta-secretase inhibitors for the treatment of Alzheimer's disease)

RN 849622-98-6 ZCAPLUS
CN Benzamide, 3-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.

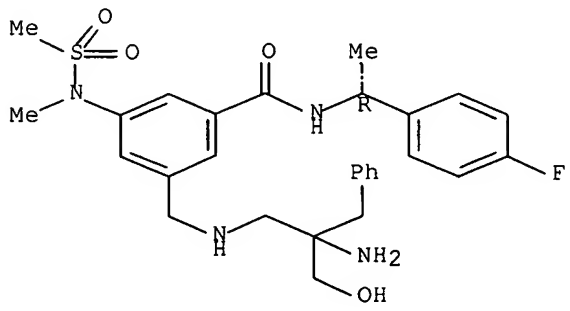


RN 849623-02-5 ZCAPLUS
CN Benzamide, 3-[[[2-amino-2-(hydroxymethyl)-3-phenylpropyl]amino]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

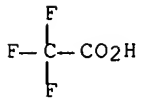
CRN 849623-01-4
CMF C28 H35 F N4 O4 S

Absolute stereochemistry.

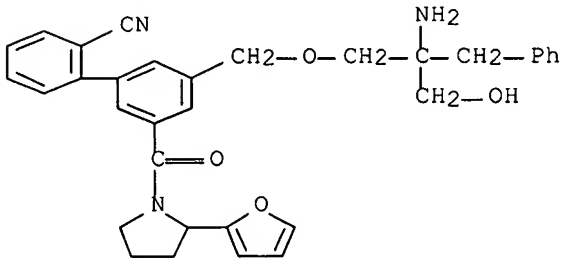


CM 2

CRN 76-05-1
CMF C2 H F3 O2

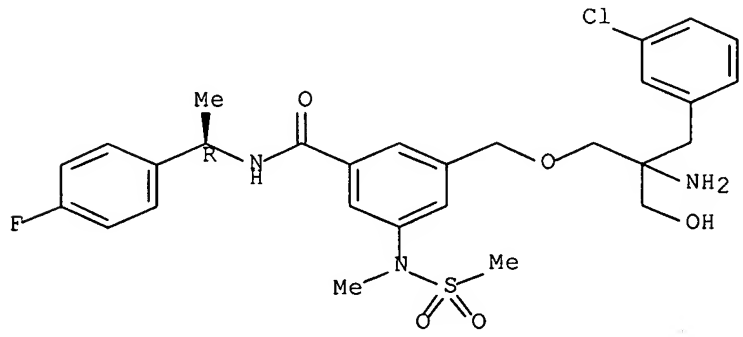


RN 849623-03-6 ZCAPLUS
CN [1,1'-Biphenyl]-2-carbonitrile, 3'-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-5'-[[2-(2-furanyl)-1-pyrrolidinyl]carbonyl]- (CA INDEX NAME)



RN 849623-05-8 ZCAPLUS
CN Benzamide, 3-[[2-amino-3-(3-chlorophenyl)-2-(hydroxymethyl)propoxy]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]- (CA INDEX NAME)

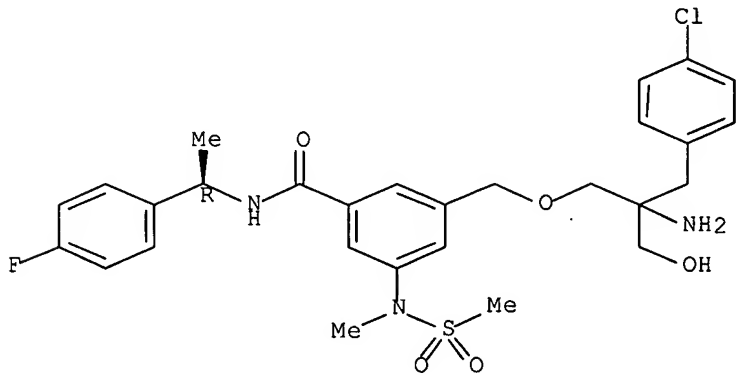
Absolute stereochemistry.



RN 849623-06-9 ZCAPLUS

CN Benzamide, 3-[[2-amino-3-(4-chlorophenyl)-2-(hydroxymethyl)propoxy]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]- (CA INDEX NAME)

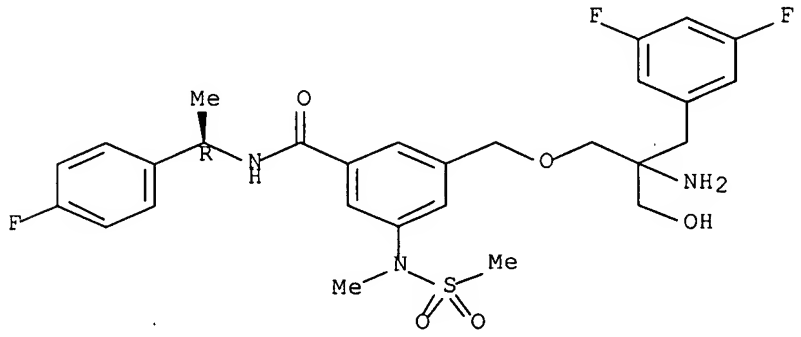
Absolute stereochemistry.



RN 849623-07-0 ZCAPLUS

CN Benzamide, 3-[[2-amino-3-(3,5-difluorophenyl)-2-(hydroxymethyl)propoxy]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]- (CA INDEX NAME)

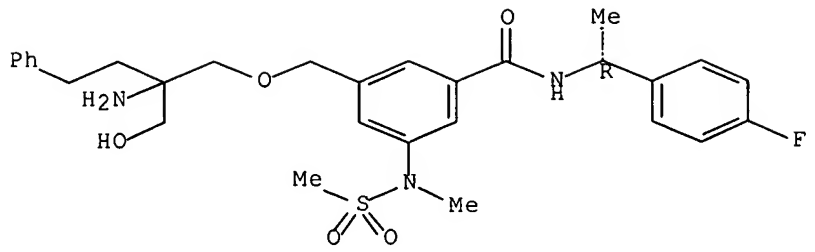
Absolute stereochemistry.



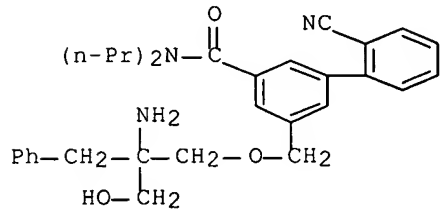
RN 849623-08-1 ZCAPLUS

CN Benzamide, 3-[[2-amino-2-(hydroxymethyl)-4-phenylbutoxy]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]- (CA INDEX NAME)

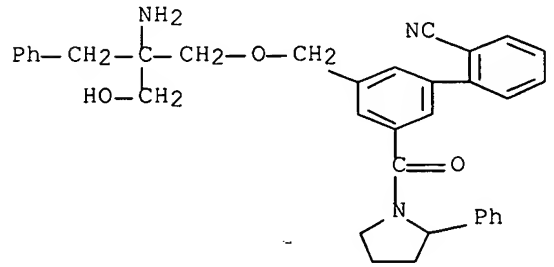
Absolute stereochemistry.



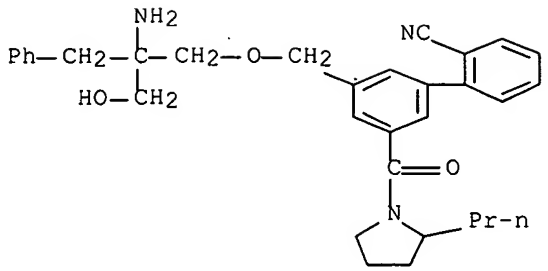
RN 849623-09-2 ZCAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 5-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-2'-cyano-N,N-dipropyl- (CA INDEX NAME)



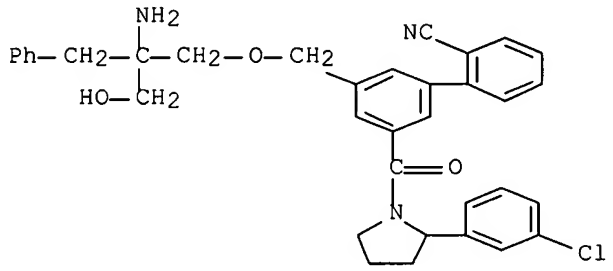
RN 849623-10-5 ZCAPLUS
CN [1,1'-Biphenyl]-2-carbonitrile, 3'-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-5'-[(2-phenyl-1-pyrrolidinyl)carbonyl]- (CA INDEX NAME)



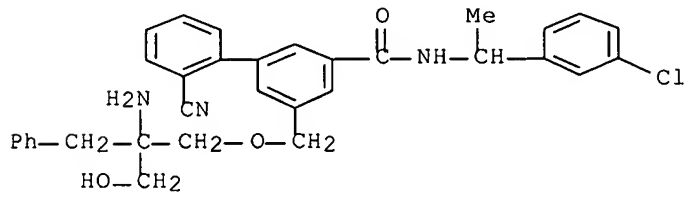
RN 849623-11-6 ZCAPLUS
CN [1,1'-Biphenyl]-2-carbonitrile, 3'-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-5'-[(2-propyl-1-pyrrolidinyl)carbonyl]- (CA INDEX NAME)



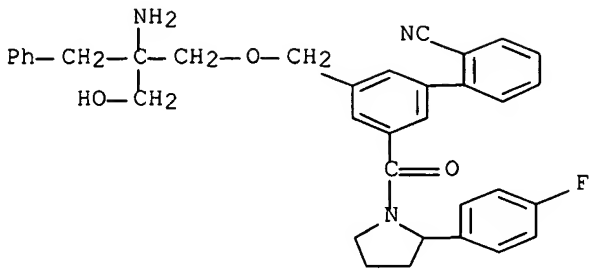
RN 849623-12-7 ZCAPLUS
CN [1,1'-Biphenyl]-2-carbonitrile, 3'-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-5'-[[2-(3-chlorophenyl)-1-pyrrolidinyl]carbonyl]- (CA INDEX NAME)



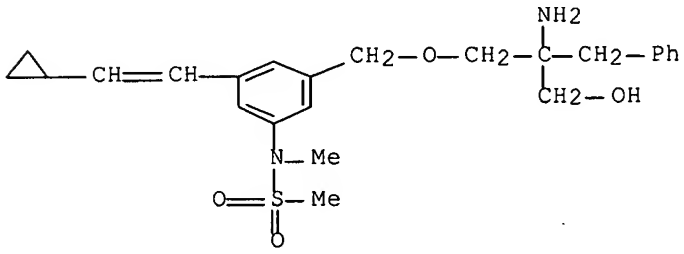
RN 849623-13-8 ZCAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 5-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-N-[1-(3-chlorophenyl)ethyl]-2'-cyano- (CA INDEX NAME)



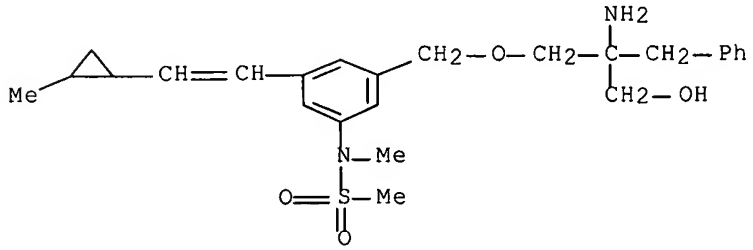
RN 849623-14-9 ZCAPLUS
CN [1,1'-Biphenyl]-2-carbonitrile, 3'-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-5'-[[2-(4-fluorophenyl)-1-pyrrolidinyl]carbonyl]- (CA INDEX NAME)



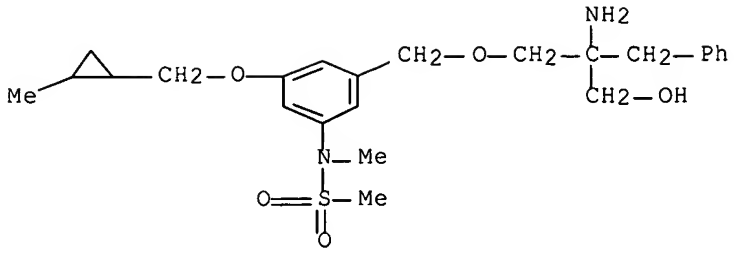
RN 849623-15-0 ZCAPLUS
CN Methanesulfonamide, N-[3-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-5-(2-cyclopropylethenyl)phenyl]-N-methyl- (CA INDEX NAME)



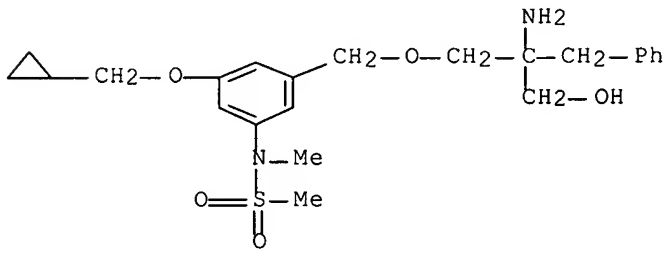
RN 849623-16-1 ZCAPLUS
CN Methanesulfonamide, N-[3-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-5-[2-(2-methylcyclopropyl)ethenyl]phenyl]-N-methyl- (CA INDEX NAME)



RN 849623-18-3 ZCAPLUS
CN Methanesulfonamide, N-[3-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-5-[(2-methylcyclopropyl)methoxy]phenyl]-N-methyl- (CA INDEX NAME)



RN 849623-19-4 ZCAPLUS
CN Methanesulfonamide, N-[3-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-5-(cyclopropylmethoxy)phenyl]-N-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 7 ZCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2005:55021 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:134323
TITLE: Preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease
INVENTOR(S): Nantermet, Philippe G.; Rajapakse, Hemaka Anthony; Selnick, Harold G.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005004803 | A2 | 20050120 | WO 2004-US20525 | 20040625 |
| WO 2005004803 | A3 | 20050421 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

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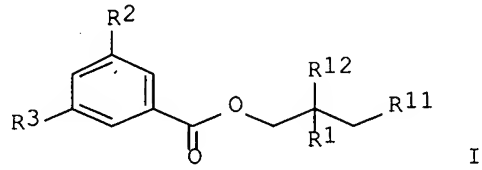
| AU 2004255191 | A1 | 20050120 | AU 2004-255191 | 20040625 |
| CA 2530006 | A1 | 20050120 | CA 2004-2530006 | 20040625 |
| EP 1643986 | A2 | 20060412 | EP 2004-756168 | 20040625 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK | | | | |
| CN 1909897 | A | 20070207 | CN 2004-80018651 | 20040625 |
| JP 2007522088 | T | 20070809 | JP 2006-518686 | 20040625 |
| IN 2005DN05946 | A | 20080509 | IN 2005-DN5946 | 20051220 |
| US 20060149092 | A1 | 20060706 | US 2005-562470 | 20051222 |
| US 7348448 | B2 | 20080325 | | |

PRIORITY APPLN. INFO.: US 2003-484150P P 20030701
WO 2004-US20525 W 20040625

OTHER SOURCE(S): MARPAT 142:134323
GI

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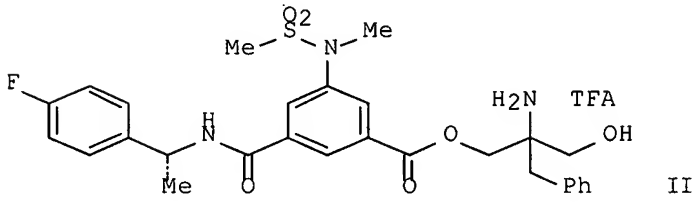



II

AB Title compds. [I; R1, R5, R9, R10 = H, (substituted) alkyl, alkenyl, alkynyl; R2 = R4SO2NR7, (substituted) Ph; R4 = (substituted) alkyl, alkenyl, alkynyl, Ph, PhCH2; R7 = H, alkyl, alkenyl, alkynyl; R3 = (substituted) PhCHR5NHCO, R9R10NHCO, etc.; R9R10 = atoms to form (substituted) pyrrolidinyl, piperidinyl; R11 = OH, alkoxy, phenylalkoxy, PhO, Ph; R12 = NR9R10, OH], were prepared as β-secretase inhibitors for the treatment of Alzheimer's disease (no data). Title compound (II) was prepared in several steps.

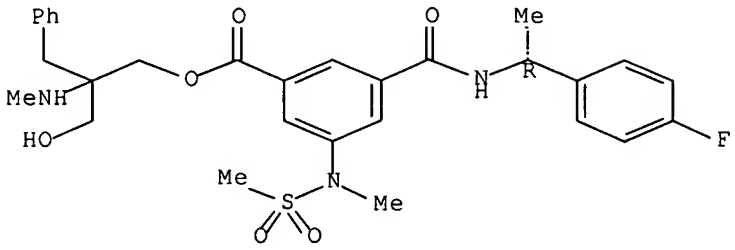
IT **827039-49-6P** **827039-54-3P** **827039-55-4P**
**827039-57-6P** **827039-58-7P** **827039-59-8P**
**827039-60-1P** **827039-61-2P** **827039-62-3P**
**827039-63-4P** **827039-64-5P** **827039-65-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease)

RN 827039-49-6 ZCAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-

[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-(methylamino)-2-(phenylmethyl)propyl ester (9CI) (CA INDEX NAME)

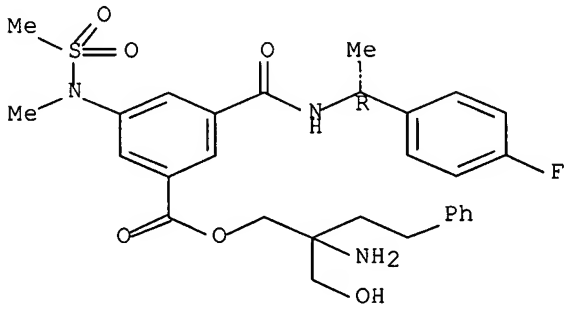
Absolute stereochemistry.



RN 827039-54-3 ZCAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(hydroxymethyl)-4-phenylbutyl ester (CA INDEX NAME)

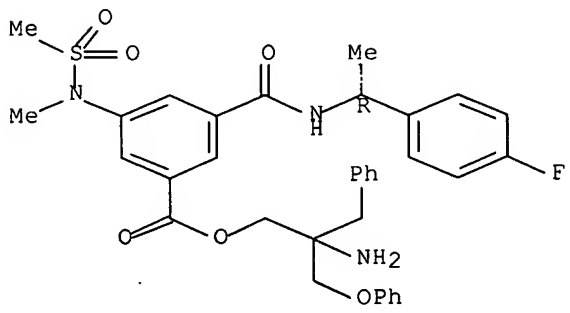
Absolute stereochemistry.



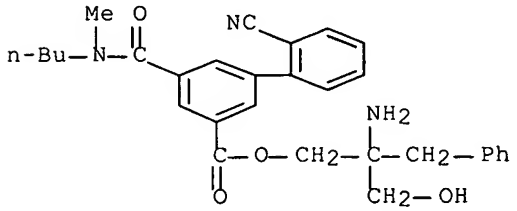
RN 827039-55-4 ZCAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(phenoxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

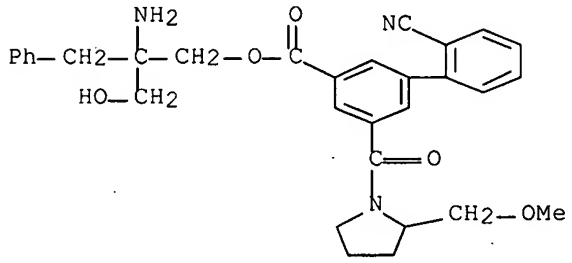
Absolute stereochemistry.



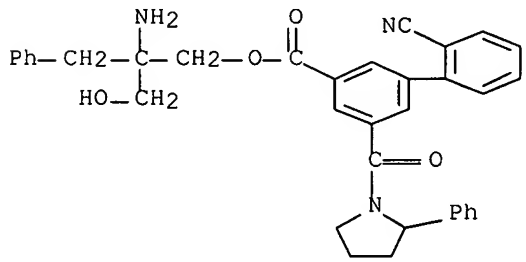
RN 827039-57-6 ZCAPLUS
CN [1,1'-Biphenyl]-3-carboxylic acid,
5-[(butylmethylamino)carbonyl]-2'-cyano-,
2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)



RN 827039-58-7 ZCAPLUS
CN [1,1'-Biphenyl]-3-carboxylic acid,
2'-cyano-5-[[2-(methoxymethyl)-1-pyrrolidinyl]carbonyl]-,
2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)



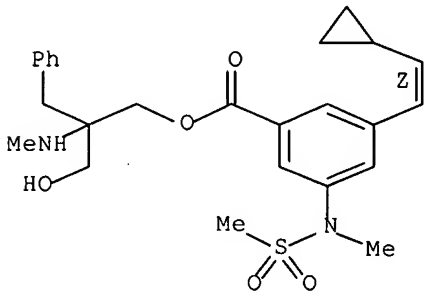
RN 827039-59-8 ZCAPLUS
CN [1,1'-Biphenyl]-3-carboxylic acid,
2'-cyano-5-[(2-phenyl-1-pyrrolidinyl)carbonyl]-,
2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)



RN 827039-60-1 ZCAPLUS
CN Benzoic acid, 3-[(1Z)-2-cyclopropylethenyl]-5-

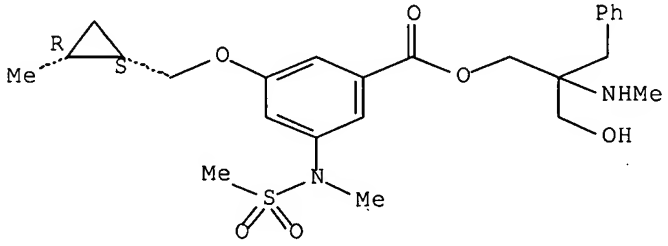
[methyl(methylsulfonyl)amino]-, 2-(hydroxymethyl)-2-(methylamino)-3-phenylpropyl ester (CA INDEX NAME)

Double bond geometry as shown.

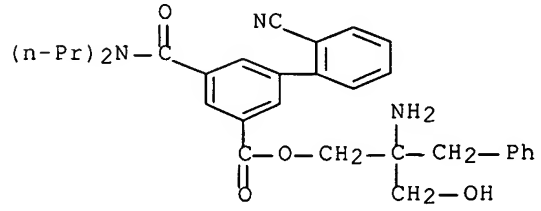



RN 827039-61-2 ZCAPLUS
CN Benzoic acid, 3-[[(1R,2S)-2-methylcyclopropyl]methoxy]-5-[methyl(methylsulfonyl)amino]-, 2-(hydroxymethyl)-2-(methylamino)-3-phenylpropyl ester, rel- (CA INDEX NAME)

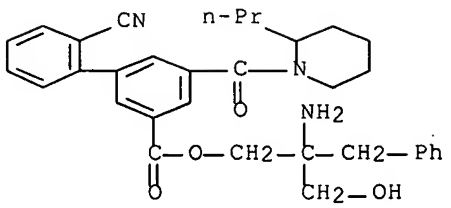
Relative stereochemistry.



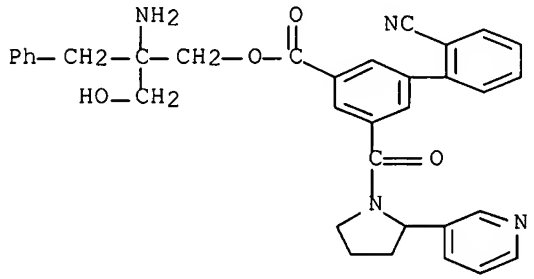

RN 827039-62-3 ZCAPLUS
CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-cyano-5-[(dipropylamino)carbonyl]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)




RN 827039-63-4 ZCAPLUS
CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-cyano-5-[(2-propyl-1-piperidinyl)carbonyl]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

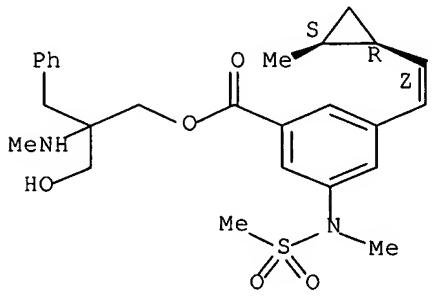


RN 827039-64-5 ZCAPLUS
CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-cyano-5-[[2-(3-pyridinyl)-1-pyrrolidinyl]carbonyl]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)



RN 827039-65-6 ZCAPLUS
CN Benzoic acid, 3-[(1Z)-2-[(1R,2S)-2-methylcyclopropyl]ethenyl]-5-[methyl(methylsulfonyl)amino]-, 2-(hydroxymethyl)-2-(methylamino)-3-phenylpropyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



IT **827039-74-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease)

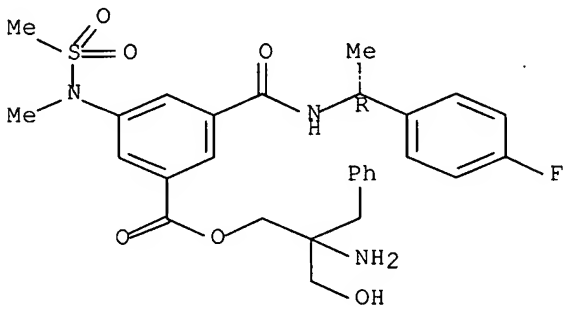
RN 827039-74-7 ZCAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

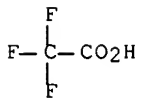
CRN 827039-73-6
CMF C28 H32 F N3 O6 S

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L17 ANSWER 3 OF 7 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:1191598 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:116781
TITLE: Discovery of Oxadiazoyl Tertiary Carbinamine Inhibitors of β-Secretase (BACE-1)
AUTHOR(S): Rajapakse, Hemaka A.; Nantermet, Philippe G.; Selnick, Harold G.; Munshi, Sanjeev; McGaughey, Georgia B.; Lindsley, Stacey R.; Young, Mary Beth; Lai, Ming-Tain; Espeseth, Amy S.; Shi, Xiao-Ping; Colussi, Dennis; Pietrak, Beth; Crouthamel, Ming-Chih; Tugusheva, Katherine; Huang, Qian; Xu, Min; Simon, Adam J.; Kuo, Lawrence; Hazuda, Daria J.; Graham, Samuel; Vacca, Joseph P.

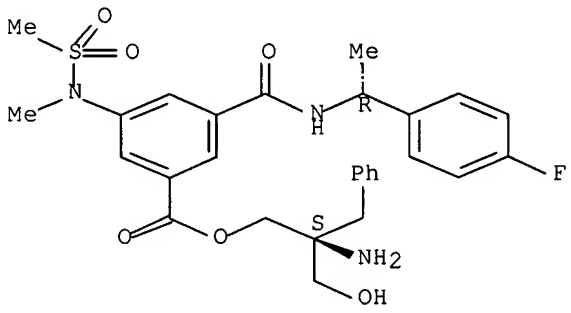
CORPORATE SOURCE: Departments of Medicinal Chemistry, Structural Biology, Molecular Systems and Alzheimer's Research, Merck Research Laboratories, West Point, PA, 19486, USA
SOURCE: Journal of Medicinal Chemistry (2006), 49(25), 7270-7273
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:116781

AB We describe the discovery and optimization of tertiary carbinamine derived inhibitors of the enzyme β-secretase (BACE-1). These novel non-transition-state-derived ligands incorporate a single primary amine to interact with the catalytic aspartates of the target enzyme. Optimization of this series provided inhibitors with intrinsic and functional potency comparable to evolved transition state isostere derived inhibitors of BACE-1.

IT **918344-77-1** **918344-77-1D**, complexes with β-secretase
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(discovery of oxadiazoyl tertiary carbinamine inhibitors of β-secretase)

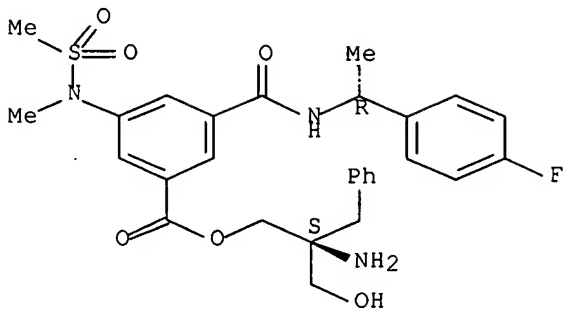
RN 918344-77-1 ZCAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, (2S)-2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.



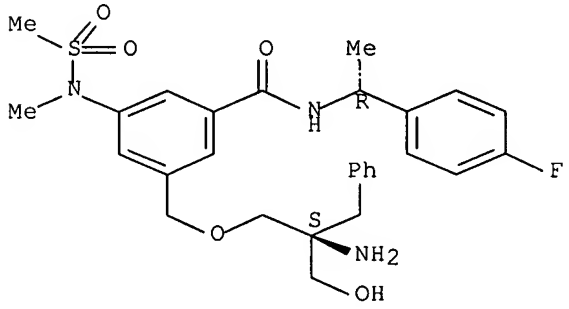
RN 918344-77-1 ZCAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, (2S)-2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.



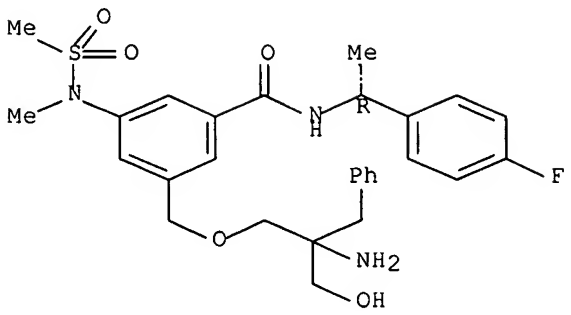
IT **905283-15-0P**
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(discovery of oxadiazoyl tertiary carbinamine inhibitors of β-secretase)
RN 905283-15-0 ZCAPLUS
CN Benzamide, 3-[[(2S)-2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.



IT **849622-98-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(discovery of oxadiazoyl tertiary carbinamine inhibitors of β-secretase)
RN 849622-98-6 ZCAPLUS
CN Benzamide, 3-[[2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 24 THERE ARE 24 CAPLUS RECORDS THAT CITE THIS RECORD (24 CITINGS)
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

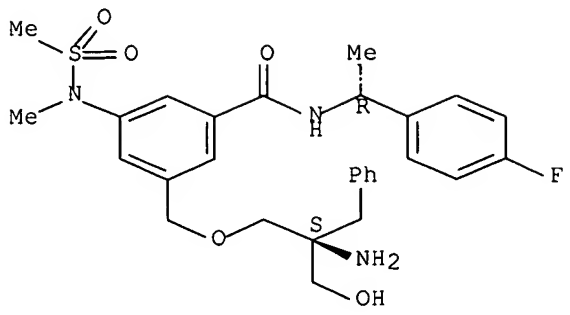
L17 ANSWER 4 OF 7 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:502466 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:224304
TITLE: Computational approaches to the prediction of blood-brain barrier permeability: a comparative analysis of central nervous system drugs versus secretase inhibitors for Alzheimer's disease
AUTHOR(S): Rishton, Gilbert M.; LaBonte, Kristen; Williams, Antony J.; Kassam, Karim; Kolovanov, Eduard
CORPORATE SOURCE: Channel Islands Alzheimer's Institute, California State University Channel Islands, Camarillo, CA, 93012, USA
SOURCE: Current Opinion in Drug Discovery & Development (2006), 9(3), 303-313
CODEN: CODDFF; ISSN: 1367-6733
PUBLISHER: Thomson Scientific
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This review summarizes progress made in the development of fully computational approaches to the prediction of blood-brain barrier (BBB) permeability of small mols., with a focus on rapid computational methods suitable for the anal. of large compound sets and virtual screening. A comparative anal. using the recently developed Advanced Chemical Development (ACD/Labs) Inc BBB permeability algorithm for the calcn. of logBB values for known Alzheimer's disease medicines, selected central nervous system drugs and new secretase inhibitors for Alzheimer's disease, is presented. The trends in logBB values and the associated physiochem. properties of these agents as they relate to the potential for BBB permeability are also discussed.

IT **905283-15-0**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(computational approaches to prediction of blood-brain barrier permeability and comparative anal. of central nervous system drugs vs. secretase inhibitors for Alzheimer's disease)

RN 905283-15-0 ZCAPLUS
CN Benzamide, 3-[[(2S)-2-amino-2-(hydroxymethyl)-3-phenylpropoxy]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.



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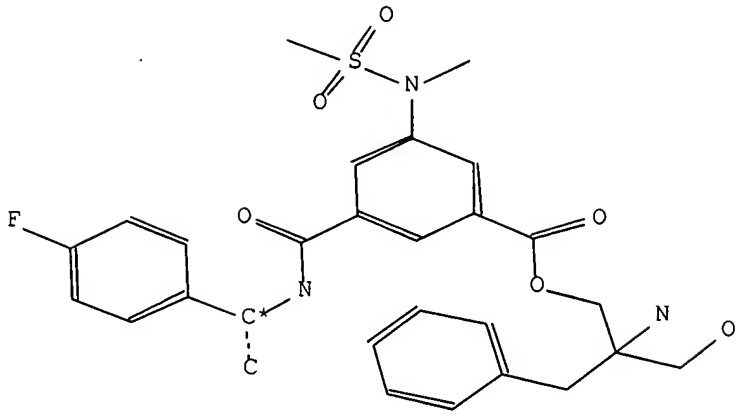
|---|---|---|
| OS.CITING REF COUNT: | 9 | THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS) |
| REFERENCE COUNT: | 77 | THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT |

L17 ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2009 Elsevier Inf. Sys. on STN

| | |
|---|---|
| Beilstein Records (BRN): | 10738675 |
| Chemical Name (CN): | 2-amino-2-benzyl-3-hydroxypropyl 3-(<<(1R)-1-(4-fluorophenyl)ethyl>amino>-carbonyl)-5-<methyl(methylsulfonyl)amino>benzoate |
| Autonom Name (AUN): | N-<1-(4-fluoro-phenyl)-ethyl>-5-(methanesulfonyl-methyl-amino)-isophthalamic acid 2-amino-2-hydroxymethyl-3-phenyl-propyl ester |
| Molec. Formula (MF): | C28 H32 F N3 O6 S |
| Molecular Weight (MW): | 557.64 |
| Lawson Number (LN): | 16137, 15201, 14151, 2817, 2705 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | isocyclic |
| Constitution ID (CONSID): | 8993254 |
| Entry Date (DED): | 2007/07/13 |
| Update Date (DUPD): | 2007/07/13 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 5 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| NMR | Nuclear Magnetic Resonance | 2 |
| PHARM | Pharmacological Data | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

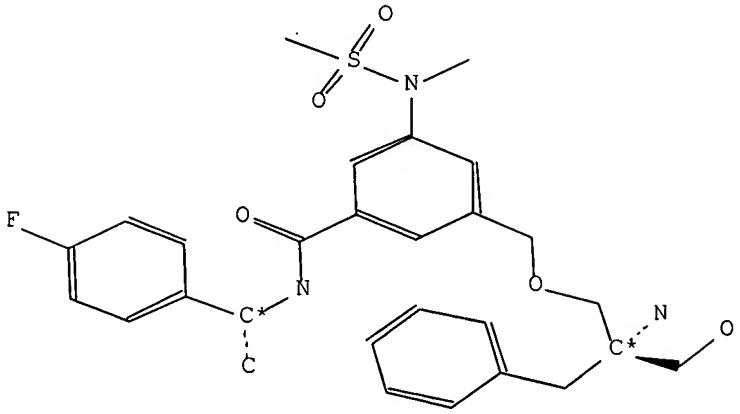
All References:
ALLREF

1. Rajapakse, Hemaka A.; Nantermet, Philippe G.; Selnick, Harold G.; Munshi, Sanjeev; McGaughey, Georgia B.; Lindsley, Stacey R.; Young, Mary Beth; Lai, Ming-Tain; Espeseth, Amy S.; Shi, Xiao-Ping; Colussi, Dennis; et al., J. Med. Chem., CODEN: JMCMAR, SIR49(25), <2006>, 7270 - 7273; BABS-6653343

L17 ANSWER 6 OF 7 BEILSTEIN COPYRIGHT 2009 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 10737733
Chemical Name (CN): 3-<((S)-2-amino-2-benzyl-3-hydroxypropyl)methyl>-N-<(1R)-1-(4-fluorophenyl)ethyl>-5-<methyl(methylsulfonyl)amino>benzamide

| | |
|---|---|
| Autonom Name (AUN): | 3-(2-amino-2-hydroxymethyl-3-phenyl-propoxymethyl)-N-<1-(4-fluoro-phenyl)-ethyl>-5-(methanesulfonyl-methyl-amino)-benzamide |
| Molec. Formula (MF): | C28 H34 F N3 O5 S |
| Molecular Weight (MW): | 543.65 |
| Lawson Number (LN): | 16184, 15201, 14151, 2817, 2705 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | isocyclic |
| Constitution ID (CONSID): | 8992434 |
| Entry Date (DED): | 2007/07/13 |
| Update Date (DUPD): | 2007/07/13 |



Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 5 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| PHARM | Pharmacological Data | 1 |

This substance also occurs in Reaction Documents:

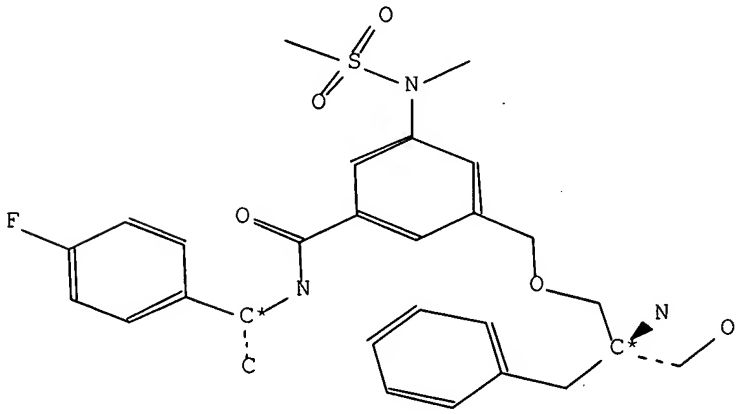
| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

All References:
ALLREF

1. Rajapakse, Hemaka A.; Nantermet, Philippe G.; Selnick, Harold G.; Munshi, Sanjeev; McGaughey, Georgia B.; Lindsley, Stacey R.; Young, Mary Beth; Lai, Ming-Tain; Espeseth, Amy S.; Shi, Xiao-Ping; Colussi, Dennis; et al., J. Med. Chem., CODEN: JMCMAR, SIR49(25), <2006>, 7270 - 7273; BABS-6653343

L17 ANSWER 7 OF 7 BEILSTEIN COPYRIGHT 2009 Elsevier Inf. Sys. on STN

| | |
|---|---|
| Beilstein Records (BRN): | 10737732 |
| Chemical Name (CN): | 3-<((R)-2-amino-2-benzyl-3-hydroxypropyl)methyl>-N-<(1R)-1-(4-fluorophenyl)ethyl>-5-<methyl(methylsulfonyl)amino>benzamide |
| Autonom Name (AUN): | 3-(2-amino-2-hydroxymethyl-3-phenyl-propoxymethyl)-N-<1-(4-fluoro-phenyl)-ethyl>-5-(methanesulfonyl-methyl-amino)-benzamide |
| Molec. Formula (MF): | C28 H34 F N3 O5 S |
| Molecular Weight (MW): | 543.65 |
| Lawson Number (LN): | 16184, 15201, 14151, 2817, 2705 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | isocyclic |
| Constitution ID (CONSID): | 8992434 |
| Entry Date (DED): | 2007/07/13 |
| Update Date (DUPD): | 2007/07/13 |




Field Availability:

| Code | Name | Occurrence |
|---|---|---|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 5 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |

| | | |
|---|---|---|
| CONSID | Constitution ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|---|---|---|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

All References:
ALLREF

1. Rajapakse, Hemaka A.; Nantermet, Philippe G.; Selnick, Harold G.; Munshi, Sanjeev; McGaughey, Georgia B.; Lindsley, Stacey R.; Young, Mary Beth; Lai, Ming-Tain; Espeseth, Amy S.; Shi, Xiao-Ping; Colussi, Dennis; et al., J. Med. Chem., CODEN: JMCMAR, SIR49(25), <2006>, 7270 - 7273; BABS-6653343

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=> d his full

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     FILE 'REGISTRY' ENTERED AT 12:47:36 ON 11 DEC 2009
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L2           0 SEA SSS SAM L1

     FILE 'STNGUIDE' ENTERED AT 12:48:51 ON 11 DEC 2009

     FILE 'REGISTRY' ENTERED AT 13:11:18 ON 11 DEC 2009
L3             SCREEN 1071
L4           3 SEA SSS SAM L1 AND L3
               D SCA
               D STAT QUE
L5          38 SEA SSS FUL L1 AND L3
               SAVE TEMP L5 WAR232L1L3/A

     FILE 'ZCAPLUS' ENTERED AT 13:13:15 ON 11 DEC 2009
L6           4 SEA SPE=ON  ABB=ON  PLU=ON  L5

     FILE 'BEILSTEIN' ENTERED AT 13:13:23 ON 11 DEC 2009
L7           0 SEA SSS SAM L1 AND L3
L8           3 SEA SSS FUL L1 AND L3

     FILE 'WPIX' ENTERED AT 13:14:06 ON 11 DEC 2009
L9           2 SEA SSS SAM L1 AND L3
L10         27 SEA SSS FUL L1 AND L3
L11          2 SEA SPE=ON  ABB=ON  PLU=ON  L10/DCR

     FILE 'MARPAT' ENTERED AT 13:18:58 ON 11 DEC 2009
L12            STRUCTURE UPLOADED
L13          3 SEA SSS SAM L12
L14            STRUCTURE UPLOADED
L15          0 SEA SSS SAM L14
L16          1 SEA SSS FUL L14
               D SCA
               D BIB

     FILE 'REGISTRY' ENTERED AT 13:24:46 ON 11 DEC 2009

     FILE 'ZCAPLUS' ENTERED AT 13:24:49 ON 11 DEC 2009
               D STAT QUE L6

     FILE 'BEILSTEIN' ENTERED AT 13:25:02 ON 11 DEC 2009
               D STAT QUE L8

     FILE 'WPIX' ENTERED AT 13:25:10 ON 11 DEC 2009
               D STAT QUE L11

     FILE 'MARPAT' ENTERED AT 13:25:20 ON 11 DEC 2009
               D STAT QUE L16

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L17          7 DUP REM L6 L8 L11 L16 (3 DUPLICATES REMOVED)
                   ANSWERS '1-4' FROM FILE ZCAPLUS
                   ANSWERS '5-7' FROM FILE BEILSTEIN
               D IBIB ABS HITSTR L17 1-4
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D IDE ALLREF L17 5-7

FILE HOME

FILE REGISTRY
Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 DEC 2009 HIGHEST RN 1196958-61-8
DICTIONARY FILE UPDATES: 10 DEC 2009 HIGHEST RN 1196958-61-8

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

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http://www.cas.org/support/stngen/stndoc/properties.html

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Dec 4, 2009 (20091204/UP).

FILE ZCAPLUS

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FILE COVERS 1907 - 11 Dec 2009 VOL 151 ISS 25
FILE LAST UPDATED: 10 Dec 2009 (20091210/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BEILSTEIN
FILE LAST UPDATED ON April 24, 2009

FILE COVERS 1779 TO 2008.
FILE CONTAINS 10,593,281 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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>>> Price change as of January 1st, 2008: Connect Time and Structure Search fees re-introduced. See HELP COST <<<

FILE WPIX
FILE LAST UPDATED: 4 DEC 2009 <20091204/UP>
MOST RECENT UPDATE: 200978 <200978/DW>
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No update date (UP) has been created for the reclassified documents, but they can be identified by specific update codes (see HELP CLA for details) <<<

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http://scientific.thomsonreuters.com/support/patents/coverage/latestupdate

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http://www.stn-international.com/DWPIAnaVist2_0608.html

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

>>> Japanese FI-TERM thesaurus in field /FCL added --> see NEWS <<<

FILE MARPAT
FILE CONTENT: 1961-PRESENT VOL 151 ISS 23 (20091204/ED)

MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 20090275099 05 NOV 2009
DE 102008019858 22 OCT 2009
EP 2110127 21 OCT 2009
JP 2009260249 05 NOV 2009
WO 2009135699 12 NOV 2009
GB 2459133 14 OCT 2009
FR 2930141 23 OCT 2009
RU 2370496 20 OCT 2009
CA 2653107 08 AUG 2009

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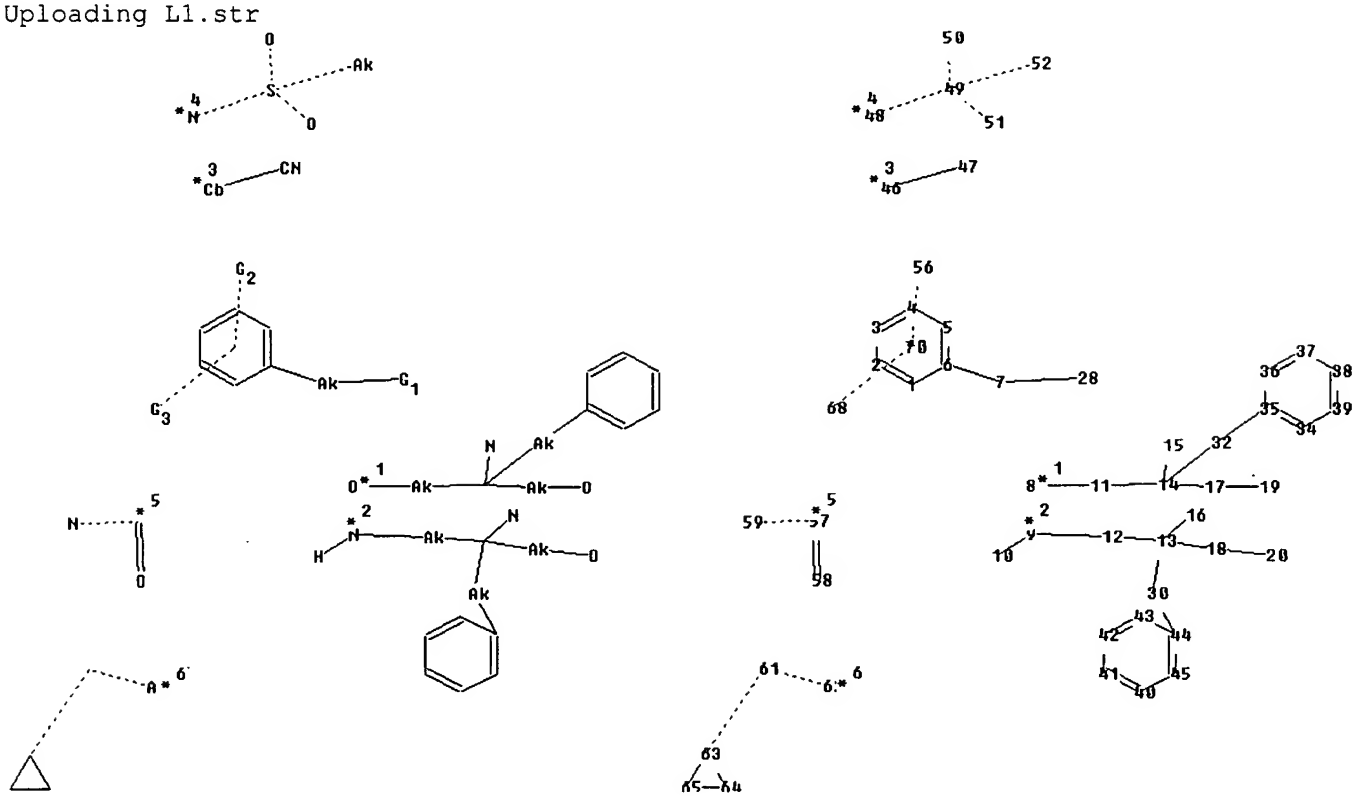

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7 8 9 10 11 12 13 14 15 16 17 18 19 20 28 30 32 46 47 48 49
50 51 52 56 57 58 61 62 68
ring nodes :
1 2 3 4 5 6 34 35 36 37 38 39 40 41 42 43 44 45 63 64 65
ring/chain nodes :
59
chain bonds :
6-7 7-28 8-11 9-10 9-12 11-14 12-13 13-16 13-18 13-30 14-15 14-17 14-32
17-19 18-20 30-44 32-35 46-47 48-49 49-50 49-51 49-52 57-58 57-59 61-62
61-63
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 34-35 34-39 35-36 36-37 37-38 38-39 40-41 40-
45
41-42 42-43 43-44 44-45 63-64 63-65 64-65

```
exact/norm bonds :
6-7  7-28  8-11  9-12  11-14  12-13  13-16  13-18  13-30  14-15  14-17  14-32  30-
44
32-35  48-49  49-50  49-51  49-52  57-58  57-59  61-62  61-63  63-64  63-65  64-65
exact bonds :
9-10  17-19  18-20  46-47
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  34-35  34-39  35-36  36-37  37-38  38-39  40-41  40-
45
41-42  42-43  43-44  44-45


G1:[*1],[*2]

G2:[*3],[*4]

G3:[*5],[*6]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS
19:CLASS  20:CLASS
28:CLASS  30:CLASS  32:CLASS  34:Atom  35:Atom  36:Atom  37:Atom  38:Atom  39:Atom
40:Atom  41:Atom
42:Atom  43:Atom  44:Atom  45:Atom  46:Atom  47:CLASS  48:CLASS  49:CLASS  50:CLASS
51:CLASS
52:CLASS  56:CLASS  57:CLASS  58:CLASS  59:CLASS  61:CLASS  62:CLASS  63:Atom
64:Atom  65:Atom
68:CLASS  69:CLASS  70:CLASS
Generic attributes :
7:
Saturation              : Saturated
11:
Saturation              : Saturated
12:
Saturation              : Saturated
17:
Saturation              : Saturated
18:
Saturation              : Saturated
30:
Saturation              : Saturated
32:
Saturation              : Saturated

Element Count :
Node 7: Limited
    C,C1-2

Node 11: Limited
    C,C1-2

Node 12: Limited
    C,C1-2

Node 17: Limited
    C,C1-2

Node 18: Limited
    C,C1-2
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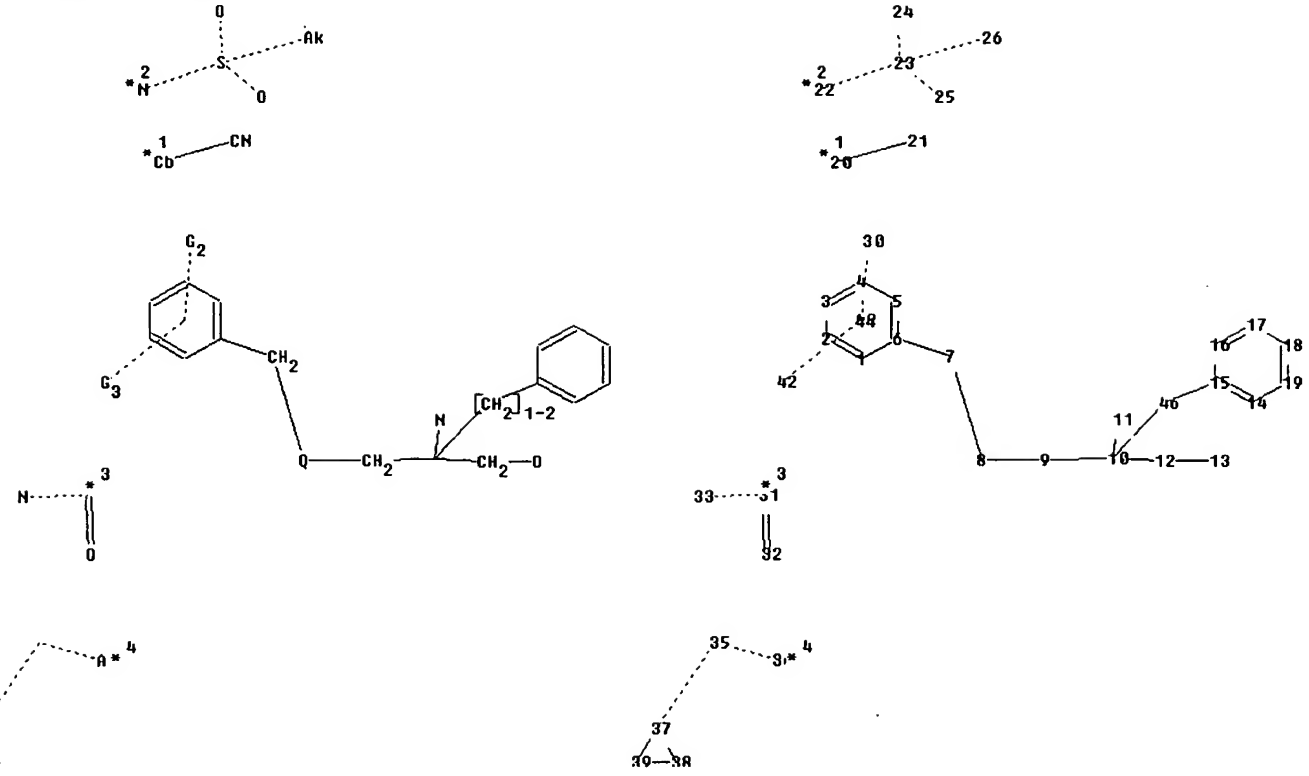
Node 30: Limited
C,C1-3

Node 32: Limited
C,C1-3

Uploading L14.str



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7 8 9 10 11 12 13 20 21 22 23 24 25 26 30 31 32 35 36 42 46

ring nodes :
1 2 3 4 5 6 14 15 16 17 18 19 37 38 39
ring/chain nodes :
33
chain bonds :
6-7 7-8 8-9 9-10 10-11 10-12 10-46 12-13 15-46 20-21 22-23 23-24 23-25
23-26 31-32 31-33 35-36 35-37
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19 37-38 37-
39
38-39
exact/norm bonds :
7-8 8-9 10-11 22-23 23-24 23-25 23-26 31-32 31-33 35-36 35-37 37-38 37-
39
38-39
exact bonds :
6-7 9-10 10-12 10-46 12-13 15-46 20-21
normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19

G2:[*1],[*2]

G3:[*3],[*4]

Connectivity :
8:2 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:CLASS
22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 30:CLASS 31:CLASS 32:Atom
33:Atom 35:CLASS 36:CLASS
37:Atom 38:Atom 39:Atom 42:CLASS 43:CLASS 44:CLASS 46:CLASS